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FILE COVERS 1907 - 10 Dec 2006 VOL 145 ISS 25
FILE LAST UPDATED: 8 Dec 2006 (20061208/ED)

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=> s de19632922/pn
L1 1 DE19632922/PN

=> d l1 iall

L1 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:126444 CAPLUS
DOCUMENT NUMBER: 128:127751
ENTRY DATE: Entered STN: 02 Mar 1998
TITLE: Process for the production of hydroxypivalic acid by the hydrogen peroxide oxidation of hydroxypivalaldehyde
INVENTOR(S): Neumann, Karl Heinz; Joentgen, Winfried; Heitkamp, Dieter; Fiege, Helmut
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 4 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
INT. PATENT CLASSIF.:
MAIN: C07C059-01
SECONDARY: C07C051-285; C07C051-235
CLASSIFICATION: 23-16 (Aliphatic Compounds)
Section cross-reference(s): 42, 45
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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NEWS 4 AUG 28 ADISCTI Reloaded and Enhanced
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NEWS 6 SEP 11 CA/CAplus enhanced with more pre-1907 records
NEWS 7 SEP 21 CA/CAplus fields enhanced with simultaneous left and right truncation
NEWS 8 SEP 25 CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS 9 SEP 25 CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 10 SEP 25 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 11 SEP 28 CEABA-VTB classification code fields reloaded with new classification scheme
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NEWS 14 OCT 23 Option to turn off MARPAT highlighting enhancements available
NEWS 15 OCT 23 CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 16 OCT 23 The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 17 OCT 30 CHEMLIST enhanced with new search and display field
NEWS 18 NOV 03 JAPIO enhanced with IPC 8 features and functionality
NEWS 19 NOV 10 CA/CAplus F-Term thesaurus enhanced
NEWS 20 NOV 10 STN Express with Discover! free maintenance release Version 8.01c now available
NEWS 21 NOV 13 CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 22 NOV 20 CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS 23 NOV 20 CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS 24 NOV 20 CA/CAplus patent kind codes will be updated
NEWS 25 DEC 01 CAS REGISTRY updated with new ambiguity codes

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

| | |
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| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|------------------|--------------|
| DE 19632922 | A1 | 19980219 | DE 1996-19632922 | 19960816 <-- |
| EP 825170 | A2 | 19980225 | EP 1997-113444 | 19970804 |
| EP 825170 | A3 | 19980415 | | |
| EP 825170 | B1 | 20010110 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, FI | | | | |
| ES 2154863 | T3 | 20010416 | ES 1997-113444 | 19970804 |
| US 5801276 | A | 19980901 | US 1997-910442 | 19970805 |
| JP 10067703 | A2 | 19980310 | JP 1997-228936 | 19970812 |
| DE 1996-19632922 | | | | A 19960816 |

PRIORITY APPLN. INFO.:

PATENT CLASSIFICATION CODES:

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|-------------|-------|---|
| DE 19632922 | ICM | C07C059-01 |
| | ICS | C07C051-285; C07C051-235 |
| | IPCI | C07C0059-01 [ICM,6]; C07C0059-00 [ICM,6,C*];
C07C0051-285 [ICS,6]; C07C0051-235 [ICS,6]; C07C0051-16
[ICS,6,C*] |
| | IPCR | C07C0051-16 [I,C*]; C07C0051-285 [I,A]; C07C0059-00
[I,C*]; C07C0059-01 [I,A] |
| EP 825170 | IPCI | C07C0059-01 [ICM,6]; C07C0059-00 [ICM,6,C*];
C07C0051-285 [ICS,6]; C07C0051-16 [ICS,6,C*] |
| | IPCR | C07C0051-16 [I,C*]; C07C0051-285 [I,A]; C07C0059-00
[I,C*]; C07C0059-01 [I,A] |
| | ECLA | C07C051/285+59/01 |
| ES 2154863 | IPCI | C07C0059-01 [ICM,7]; C07C0059-00 [ICM,7,C*];
C07C0051-285 [ICS,7]; C07C0051-16 [ICS,7,C*] |
| | IPCR | C07C0051-16 [I,C*]; C07C0051-285 [I,A]; C07C0059-00
[I,C*]; C07C0059-01 [I,A] |
| US 5801276 | IPCI | C07C0051-235 [ICM,6]; C07C0051-16 [ICM,6,C*] |
| | IPCR | C07C0051-16 [I,C*]; C07C0051-285 [I,A]; C07C0059-00
[I,C*]; C07C0059-01 [I,A] |
| | NCL | 562/531.000 |
| | ECLA | C07C051/285+59/01 |
| JP 10067703 | IPCI | C07C0059-01 [ICM,6]; C07C0059-00 [ICM,6,C*];
C07C0051-285 [ICS,6]; C07C0051-16 [ICS,6,C*] |

OTHER SOURCE(S):

CASREACT 128:127751

ABSTRACT:

Hydroxypivalic acid, useful as an industrial intermediate in the preparation of water-based lacquers (no data), is prepared in high yield and selectivity by the oxidation of hydroxypivalaldehyde at 60-80° using an aqueous H₂O₂ solution in such a manner that the concentration of H₂O₂ does not exceed 4% of the reaction mixture and

that the H₂O₂ solution addition is terminated when the hydroxypivalaldehyde concentration becomes less than 1%.

SUPPL. TERM: hydroxypivalic acid manuf; hydroxypivalaldehyde oxidn manuf
hydroxypivalic acid; hydrogen peroxide oxidn
hydroxypivalaldehyde manuf hydroxypivalic

INDEX TERM: Oxidation
(liquid-phase; of hydroxypivalaldehyde with hydrogen peroxide oxidation in the manufacture of hydroxypivalic acid)

INDEX TERM: 597-31-9P, Hydroxypivalaldehyde
ROLE: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(process for the production of hydroxypivalic acid by the hydrogen peroxide oxidation of hydroxypivalaldehyde)

INDEX TERM: 4835-90-9P, Hydroxypivalic acid
ROLE: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

INDEX TERM: (process for the production of hydroxypivalic acid by the hydrogen peroxide oxidation of hydroxypivalaldehyde)
 50-00-0, Formalin, reactions 78-84-2, Isobutyraldehyde
 7722-84-1, Hydrogen peroxide, reactions
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (process for the production of hydroxypivalic acid by the hydrogen peroxide oxidation of hydroxypivalaldehyde)
 INDEX TERM: 7732-18-5, Water, uses
 ROLE: NUU (Other use, unclassified); USES (Uses)
 (solvent; process for the production of hydroxypivalic acid by the hydrogen peroxide oxidation of hydroxypivalaldehyde)

=> file reg
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

| | SINCE FILE ENTRY | TOTAL SESSION |
|---------------------|------------------|---------------|
| FULL ESTIMATED COST | 6.86 | 7.07 |
| CA SUBSCRIBER PRICE | -0.75 | -0.75 |

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STRUCTURE FILE UPDATES: 8 DEC 2006 HIGHEST RN 915121-42-5
 DICTIONARY FILE UPDATES: 8 DEC 2006 HIGHEST RN 915121-42-5

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<http://www.cas.org/ONLINE/UG/regprops.html>

=> e Hydroxypivalic acid/cn
 E1 1 HYDROXYPIVALDEHYDE ISOBUTYRATE/CN
 E2 1 HYDROXYPIVALDEHYDE OXIME/CN
 E3 1 --> HYDROXYPIVALIC ACID/CN
 E4 1 HYDROXYPIVALIC ACID METHYL ESTER/CN
 E5 1 HYDROXYPIVALIC ACID NEOPENTYL GLYCOL ESTER/CN
 E6 1 HYDROXYPIVALIC ACID NEOPENTYL GLYCOL ESTER-ISOPHORONE DIISOCYANATE-TRIMETHYLOLPROPANE COPOLYMER/CN
 E7 1 HYDROXYPIVALIC ACID NEOPENTYL GLYCOL ESTER-MDI COPOLYMER/CN
 E8 1 HYDROXYPIVALIC ACID-1-ISOCYANATO-4 (OR 3) -(ISOCYANATOMETHYL)-1-METHYLCYCLOHEXANE COPOLYMER/CN
 E9 1 HYDROXYPIVALIC ACID-IPDI-PHTHALIC ANHYDRIDE-TRIMETHYLOLPROPANE COPOLYMER/CN
 E10 1 HYDROXYPIVALIC ACID-ISOPHTHALIC ACID-NEOPENTYL GLYCOL-NEOPENTYL GLYCOL HYDROXYPIVALATE-PRIMID QM 1260-TEREPHTHALIC ACID COPOLYMER/CN
 E11 1 HYDROXYPIVALIC ACID-ISOPHTHALIC ACID-NEOPENTYL GLYCOL-PRIMID

QM 1260-TEREPHTHALIC ACID COPOLYMER/CN
E12 1 HYDROXYPIVALIC ACID-ISOPHTHALIC ACID-NEOPENTYL GLYCOL-PRIMID
XL 552-TEREPHTHALIC ACID COPOLYMER/CN

=> s e3

L2 1 "HYDROXYPIVALIC ACID"/CN

=> d 12

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 4835-90-9 REGISTRY

ED Entered STN: 16 Nov 1984

CN Propanoic acid, 3-hydroxy-2,2-dimethyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Hydracrylic acid, 2,2-dimethyl- (6CI, 7CI, 8CI)

OTHER NAMES:

CN α,α -Dimethyl- β -hydroxypropionic acid

CN 2,2-Dimethyl-3-hydroxypropanoic acid

CN 2,2-Dimethyl-3-hydroxypropionic acid

CN 2,2-Dimethylhydracrylic acid

CN 3-Hydroxy-2,2-dimethylpropanoic acid

CN 3-Hydroxy-2,2-dimethylpropionic acid

CN Hydroxypivalic acid

CN NSC 115936

CN Oxypivalic acid

MF C5 H10 O3

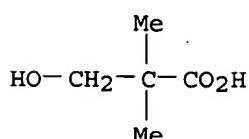
CI COM

LC STN Files: ANABSTR, BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CIN, CSCHEM, IFICDB, IFIPAT, IFIUDB, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL

(*File contains numerically searchable property data)

Other Sources: EINECS**, NDSL**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

206 REFERENCES IN FILE CA (1907 TO DATE)

64 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

206 REFERENCES IN FILE CAPLUS (1907 TO DATE)

7 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> e hydroxypivalaldehyde/cn

E1 1 HYDROXYPERIDONE/CN

E2 1 HYDROXYPIRACETAM/CN

E3 1 --> HYDROXYPIVALALDEHYDE/CN

E4 1 HYDROXYPIVALALDEHYDE DIMER/CN

E5 1 HYDROXYPIVALDEHYDE/CN

E6 1 HYDROXYPIVALDEHYDE CYANOHYDRIN/CN

E7 1 HYDROXYPIVALDEHYDE ISOBUTYRATE/CN

E8 1 HYDROXYPIVALDEHYDE OXIME/CN

E9 1 HYDROXYPIVALIC ACID/CN

E10 1 HYDROXYPIVALIC ACID METHYL ESTER/CN

E11 1 HYDROXYPIVALIC ACID NEOPENTYL GLYCOL ESTER/CN

E12 1 HYDROXYPIVALIC ACID NEOPENTYL GLYCOL ESTER-ISOPHORONE DIISOC

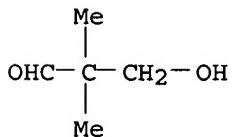
YANATE-TRIMETHYLOLPROPANE COPOLYMER/CN

=> s e3

L3 1 HYDROXYPIVALALDEHYDE/CN

=> d 13

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN 597-31-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Propanal, 3-hydroxy-2,2-dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Hydracrylaldehyde, 2,2-dimethyl- (6CI, 7CI, 8CI)
OTHER NAMES:
CN α,α -Dimethyl- β -hydroxypropionaldehyde
CN 2,2-Dimethyl-3-hydroxypropanal
CN 2,2-Dimethyl-3-hydroxypropionaldehyde
CN 2-(Hydroxymethyl)-2-methylpropanal
CN 2-(Hydroxymethyl)isobutyraldehyde
CN 3-Hydroxy-2,2-dimethylpropanal
CN 3-Hydroxy-2,2-dimethylpropionaldehyde
CN 3-Hydroxypivalaldehyde
CN Hydroxypivalaldehyde
CN Hydroxypivaldehyde
CN Pentaaldol
CN Pentaldol
MF C5 H10 O2
CI COM
LC STN Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT,
CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, HSDB*, IFICDB, IFIPAT, IFIUDB,
PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

326 REFERENCES IN FILE CA (1907 TO DATE)
10 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
326 REFERENCES IN FILE CAPLUS (1907 TO DATE)